A Distributed Approach to Data Sharing:

DSSTox Public Toxicity Database Network

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Agency Problem:

- ➢ Too many chemicals to test
- ➢ Lack of sufficient and relevant data

Inerts

Prioritize and focus limited resources on chemicals and problem areas estimated to pose greatest potential hazard

TSCA/PMN

HPV Testing Pgm

Endocrine Disruption
Testing Program

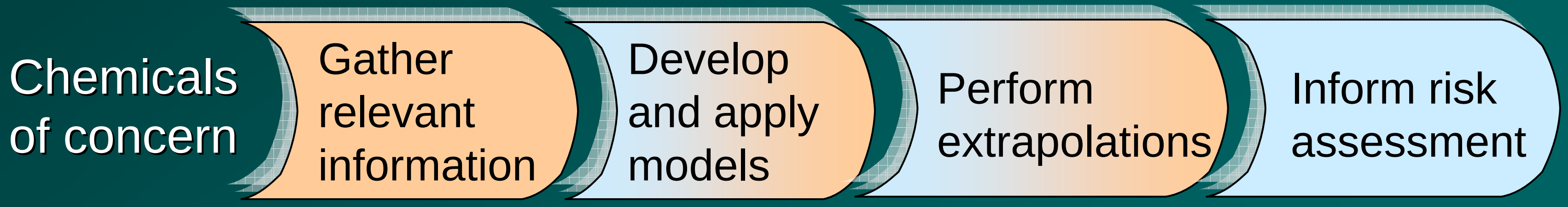
Water
CCL

Pesticides

Computational Toxicology:

The application of mathematical and computer models and molecular biological approaches to improve EPA's

- prioritization of data requirements
- risk assessments



Chemicals of concern

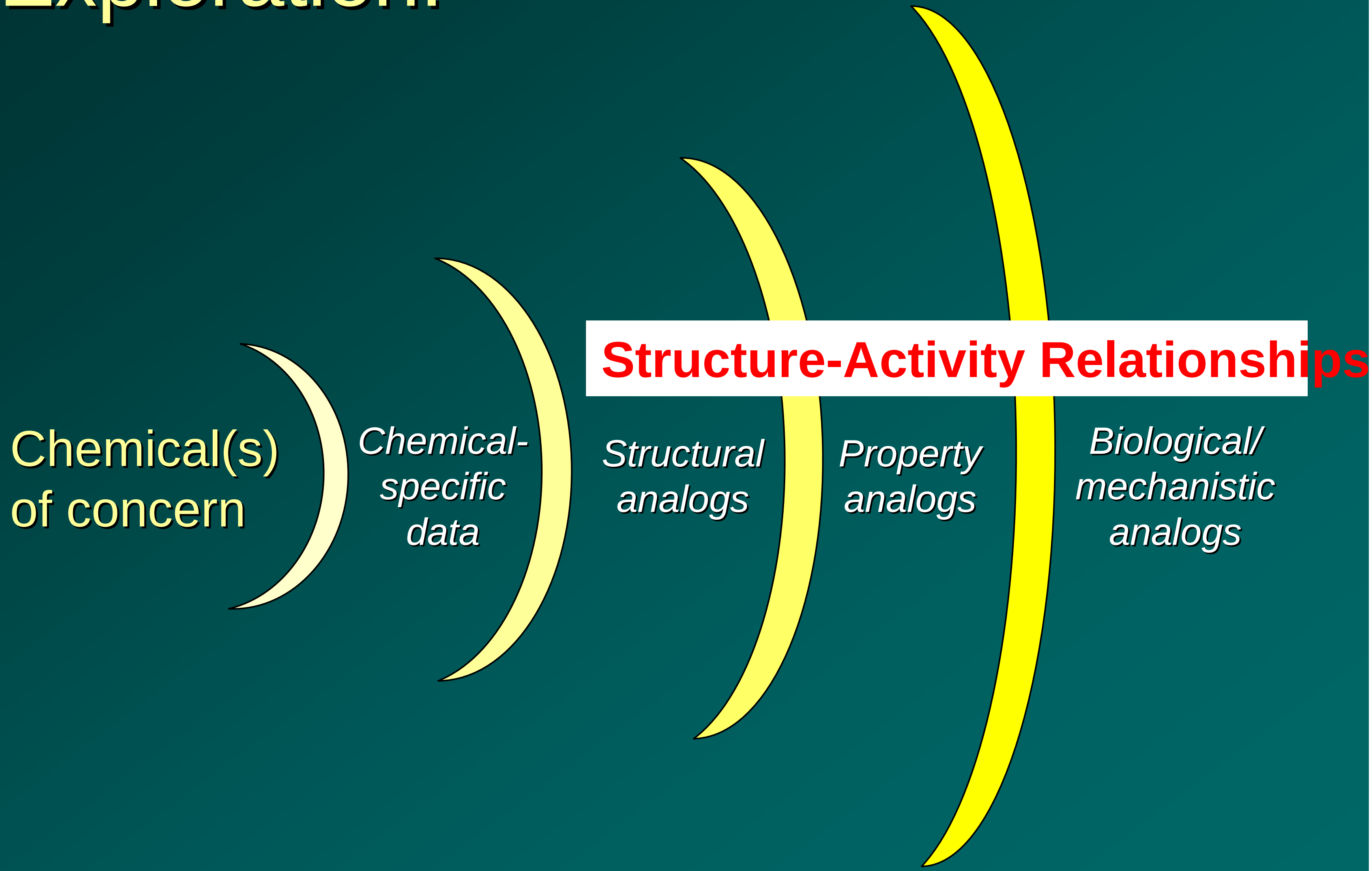
Gather relevant information

Develop and apply models

Perform extrapolations

Inform risk assessment

Chemistry-based Data Mining & Exploration:



Chemical(s) of concern

Chemical-specific data

Structure-Activity Relationships

Structural analogs

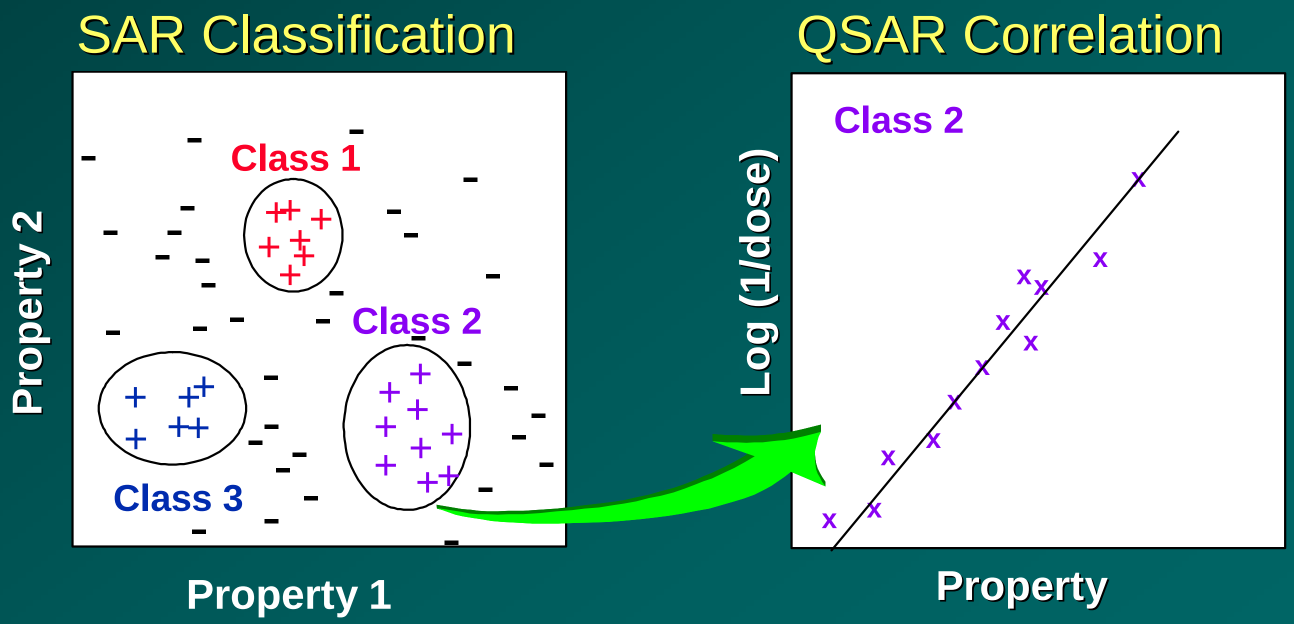
Property analogs

Biological/ mechanistic analogs

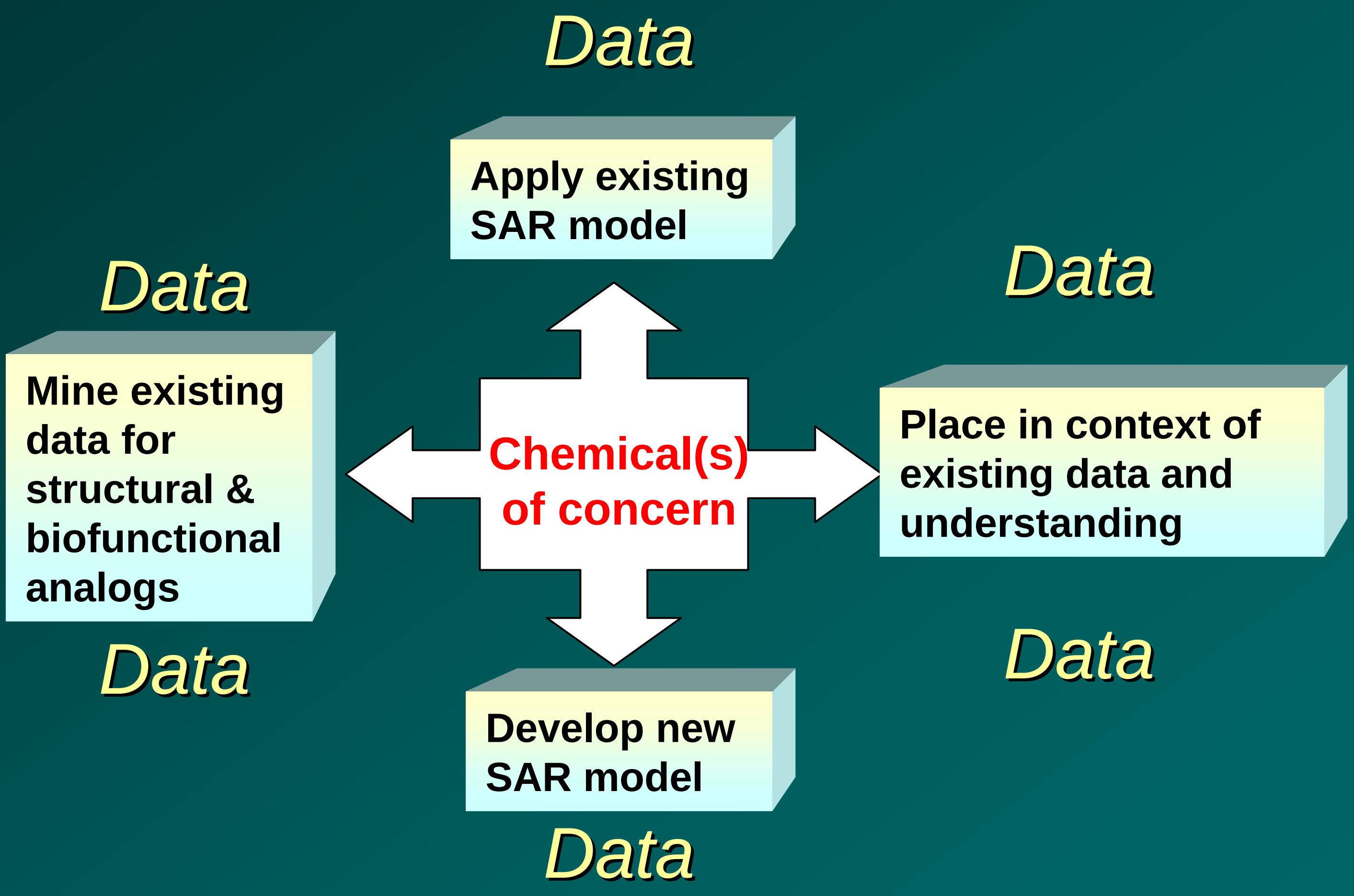
Structure-Activity Relationships (SAR):

Activity = f (structure)

Analogy
Heuristics
Machine-Learning Inference
Statistical Correlation:



Structure-based Screening & Prioritization:



Data

Apply existing SAR model

Data

Data

Mine existing data for structural & biofunctional analogs

Chemical(s) of concern

Place in context of existing data and understanding

Data

Data

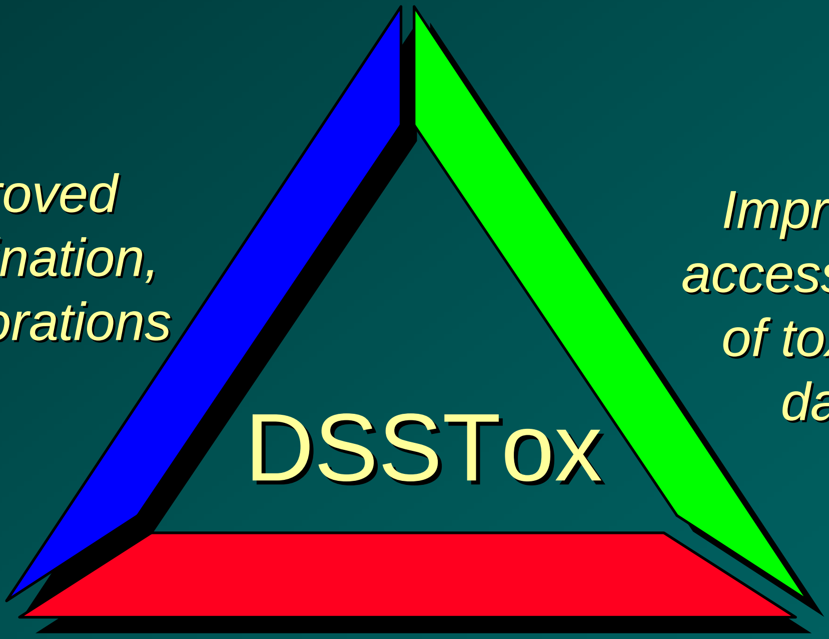
Develop new SAR model

Data

Limitations of Public Toxicity Data for Use in SAR:

- Scattered sources
- Non-standard formats
- Diverse information content
- Lack of chemical structure annotation
- Cannot access full database

Chemical structures & standardization



Improved coordination, collaborations

Improved access utility of toxicity data

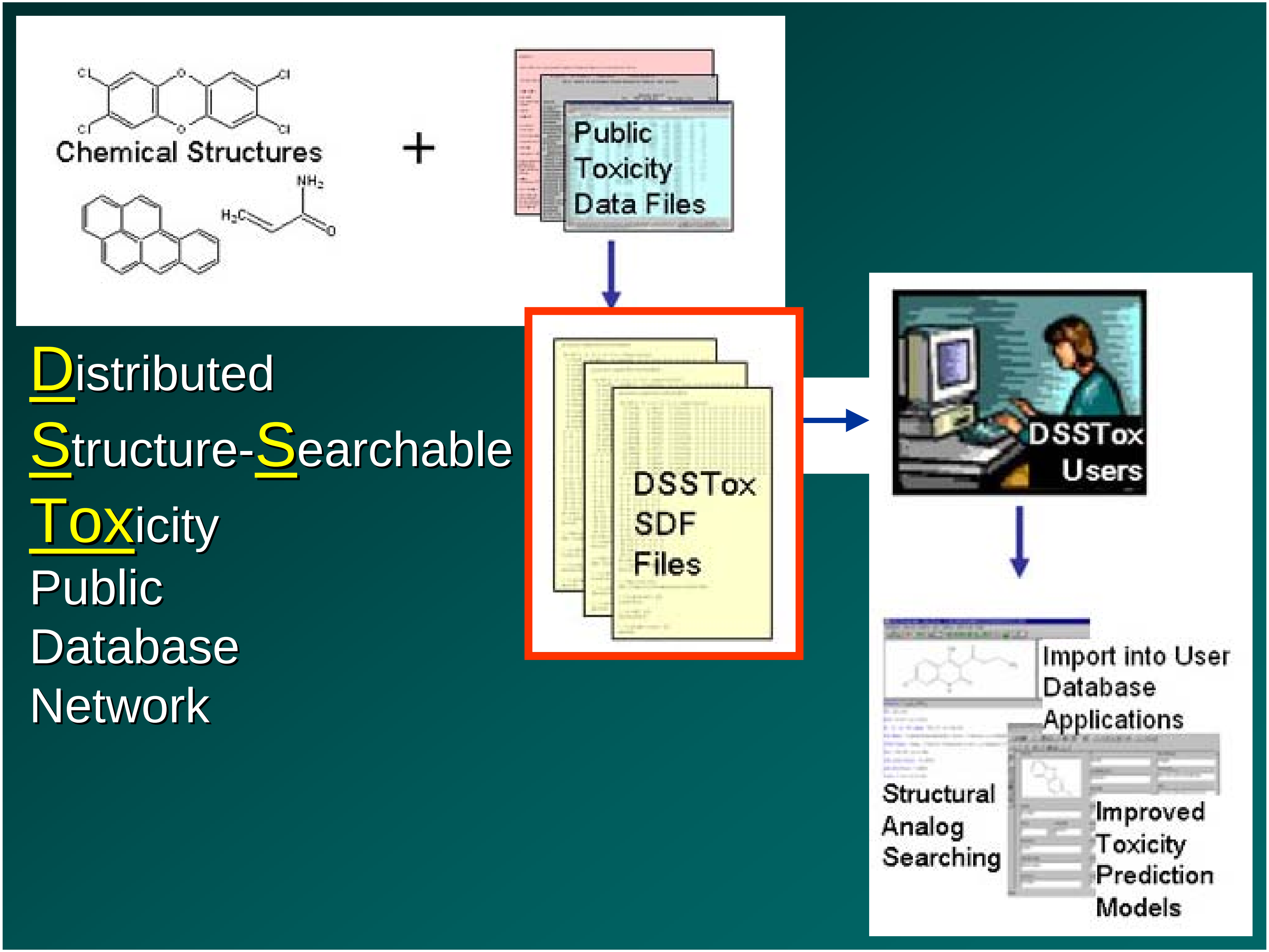
DSSTox

Open public access & partnerships

Bridging diverse toxicity disciplines

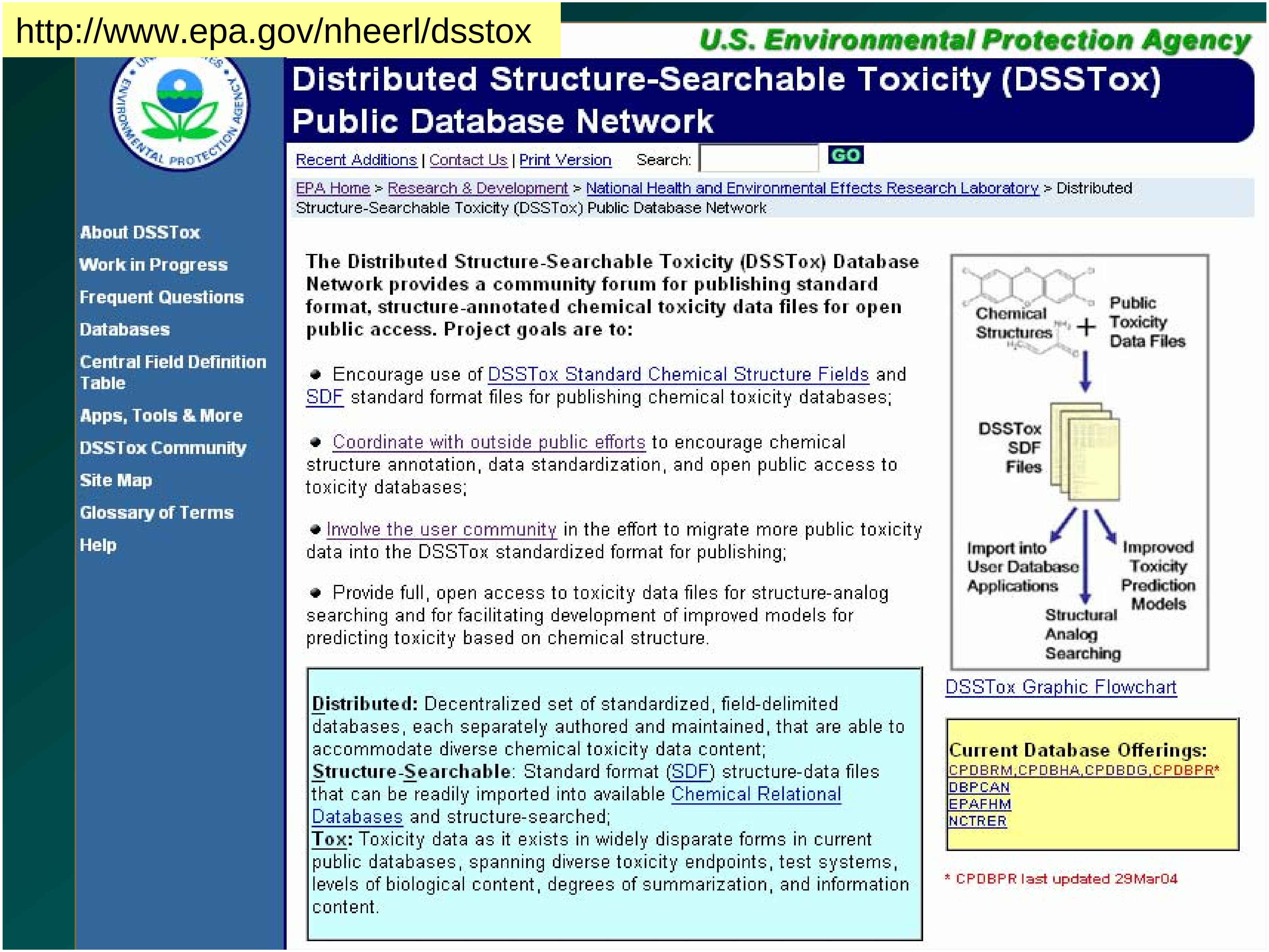
Improved toxicity prediction models

Distributed
Structure-Searchable
Toxicity
Public
Database
Network



Chemical Structures
+
Public Toxicity Data Files
DSSTox SDF Files
DSSTox Users
Import into User Database Applications
Structural Analog Searching
Improved Toxicity Prediction Models

http://www.epa.gov/nheerl/dsstox



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Import into User Database Applications
Improved Toxicity Prediction Models
Structural Analog Searching
DSSTox Graphic Flowchart

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

The Distributed Structure-Searchable Toxicity (DSSTox) Database Network provides a community forum for publishing standard format, structure-annotated chemical toxicity data files for open public access. Project goals are to:

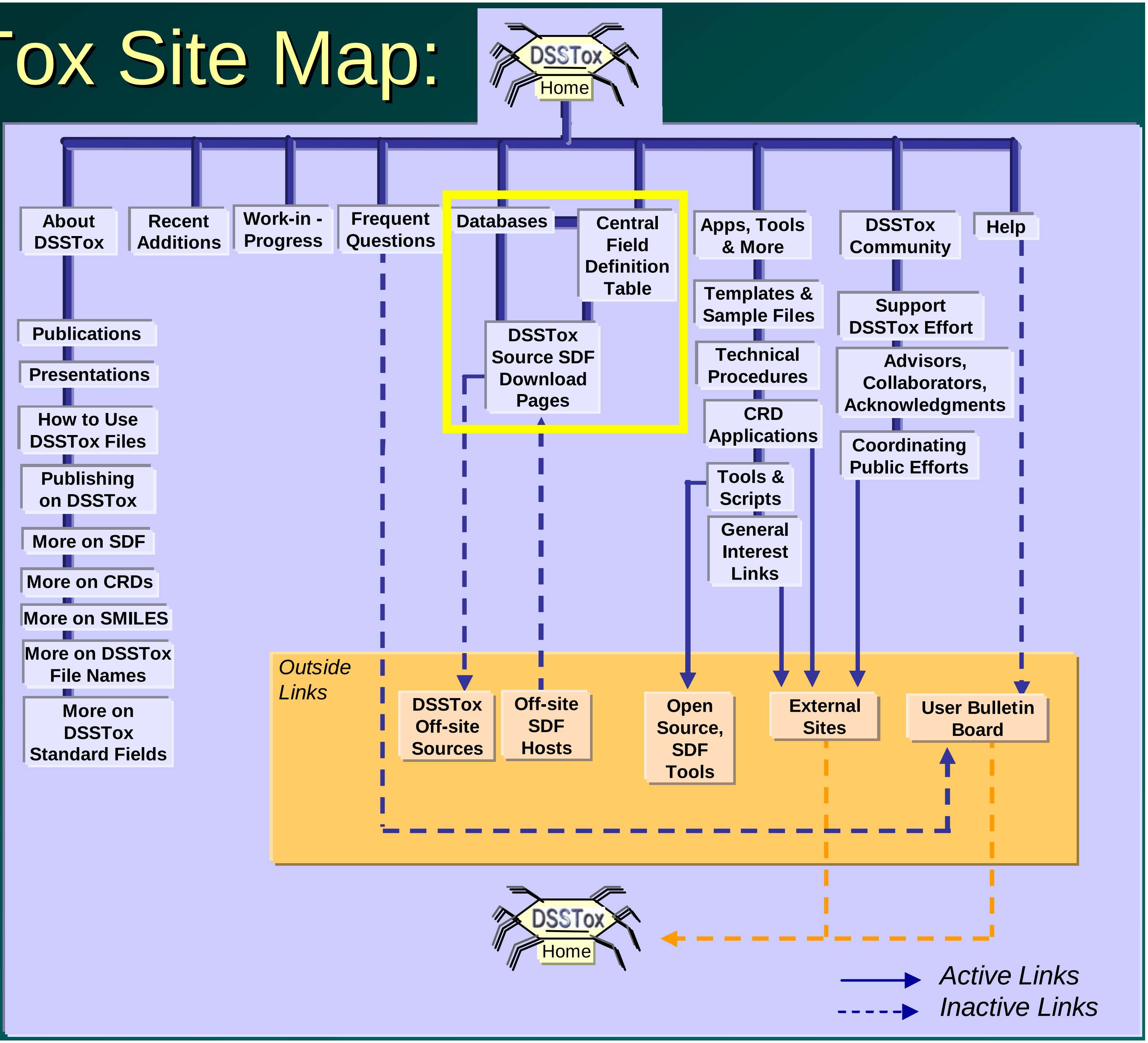
- Encourage use of DSSTox Standard Chemical Structure Fields and SDF standard format files for publishing chemical toxicity databases;
- Coordinate with outside public efforts to encourage chemical structure annotation, data standardization, and open public access to toxicity databases;
- Involve the user community in the effort to migrate more public toxicity data into the DSSTox standardized format for publishing;
- Provide full, open access to toxicity data files for structure-analog searching and for facilitating development of improved models for predicting toxicity based on chemical structure.

Distributed: Decentralized set of standardized, field-delimited databases, each separately authored and maintained, that are able to accommodate diverse chemical toxicity data content;
Structure-Searchable: Standard format (SDF) structure-data files that can be readily imported into available Chemical Relational Databases and structure-searched;
Tox: Toxicity data as it exists in widely disparate forms in current public databases, spanning diverse toxicity endpoints, test systems, levels of biological content, degrees of summarization, and information content.

Current Database Offerings:
CPDBRM,CPDBHA,CPDBDG,CPDBPR*
DBPCAN
EPAFHM
NCTRER

* CPDBPR last updated 29Mar04

DSSTox Site Map:



DSSTox Home

About DSSTox

Publications

Presentations

How to Use DSSTox Files

Publishing on DSSTox

More on SDF

More on CRDs

More on SMILES

More on DSSTox File Names

More on DSSTox Standard Fields

Recent Additions

Work-in - Progress

Frequent Questions

Databases

Central Field Definition Table

DSSTox Source SDF Download Pages

Apps, Tools & More

Templates & Sample Files

Technical Procedures

CRD Applications

Tools & Scripts

General Interest Links

DSSTox Community

Support DSSTox Effort

Advisors, Collaborators, Acknowledgments

Coordinating Public Efforts

Help

Outside Links

DSSTox Off-site Sources

Off-site SDF Hosts

Open Source, SDF Tools

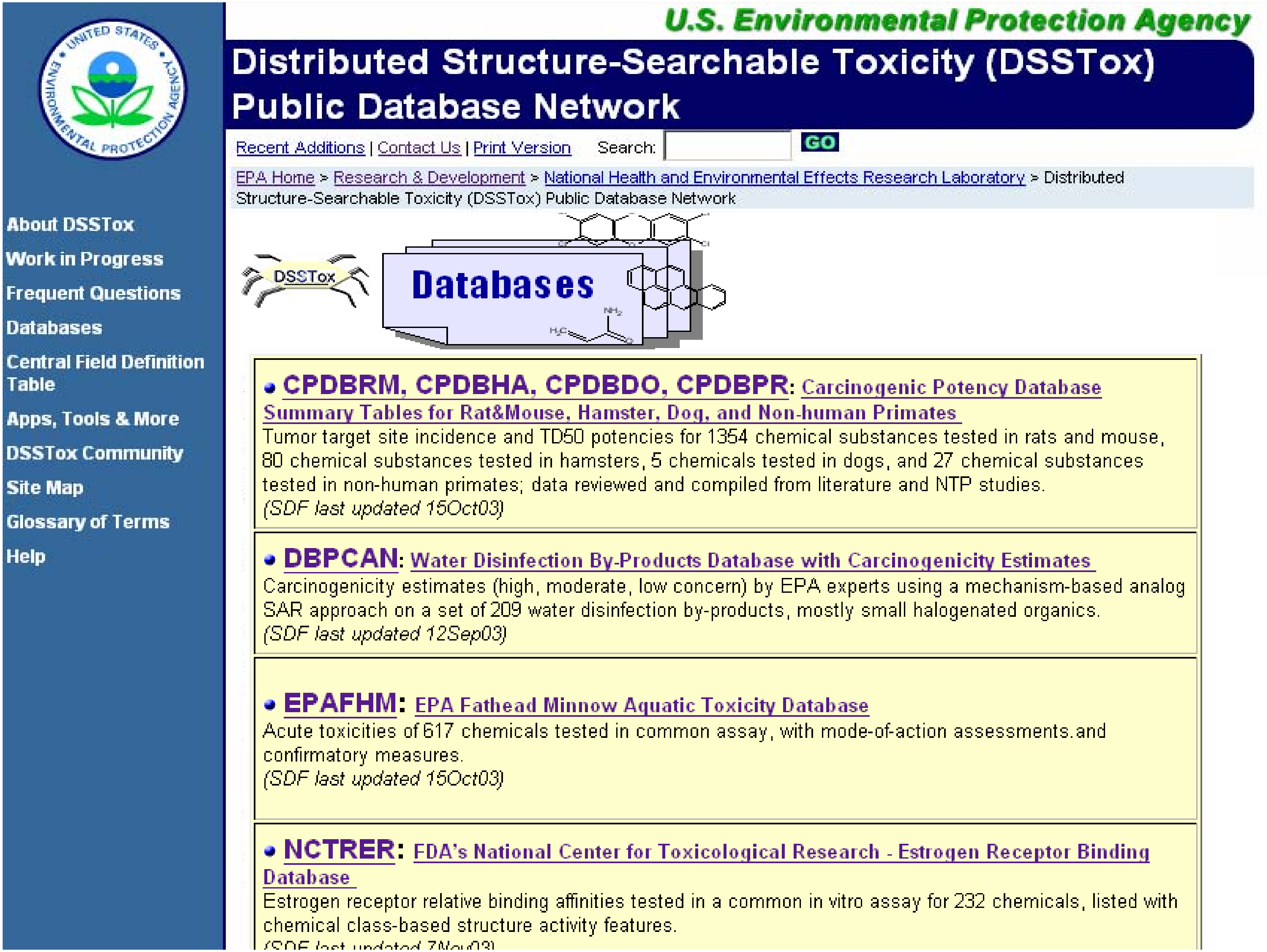
External Sites

User Bulletin Board

DSSTox Home

Active Links

Inactive Links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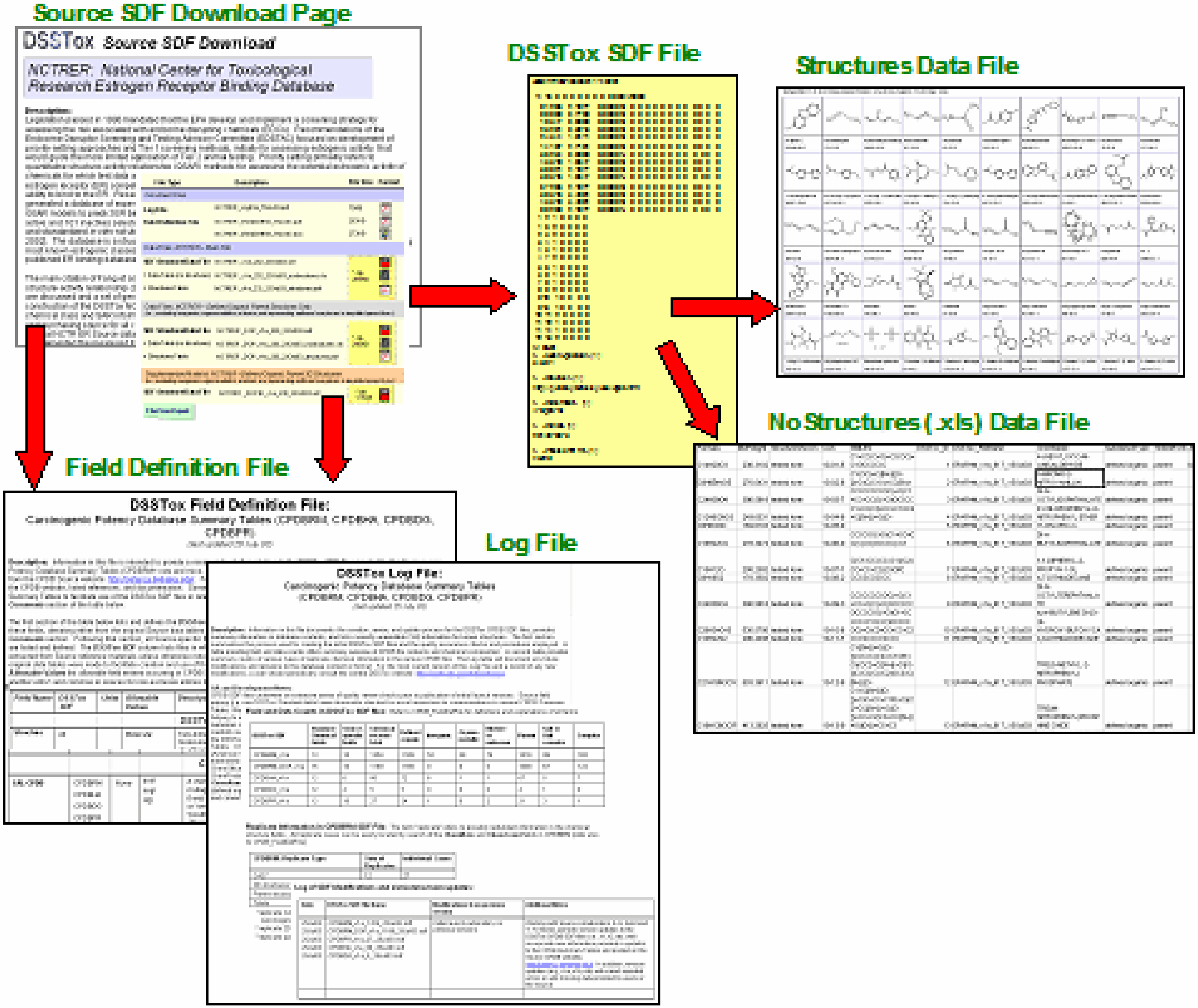
Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

- **CPDBRM, CPDBHA, CPDBDO, CPDBPR**: Carcinogenic Potency Database Summary Tables for Rat&Mouse, Hamster, Dog, and Non-human Primates
  Tumor target site incidence and TD50 potencies for 1354 chemical substances tested in rats and mouse, 80 chemical substances tested in hamsters, 5 chemicals tested in dogs, and 27 chemical substances tested in non-human primates; data reviewed and compiled from literature and NTP studies.
  (SDF last updated 15Oct03)

- **DBPCAN**: Water Disinfection By-Products Database with Carcinogenicity Estimates
  Carcinogenicity estimates (high, moderate, low concern) by EPA experts using a mechanism-based analog SAR approach on a set of 209 water disinfection by-products, mostly small halogenated organics.
  (SDF last updated 12Sep03)

- **EPAFHM**: EPA Fathead Minnow Aquatic Toxicity Database
  Acute toxicities of 617 chemicals tested in common assay, with mode-of-action assessments.and confirmatory measures.
  (SDF last updated 15Oct03)

- **NCTRER**: FDA's National Center for Toxicological Research - Estrogen Receptor Binding Database
  Estrogen receptor relative binding affinities tested in a common in vitro assay for 232 chemicals, listed with chemical class-based structure activity features.
  (SDF last updated 7Nov03)



Source SDF Download Page

DSSTox *Source SDF Download*

NCTRER: National Center for Toxicological Research Estrogen Receptor Binding Database

Description:

DSSTox SDF File

Structures Data File

No Structures (.xls) Data File

Field Definition File

DSSTox Field Definition File:

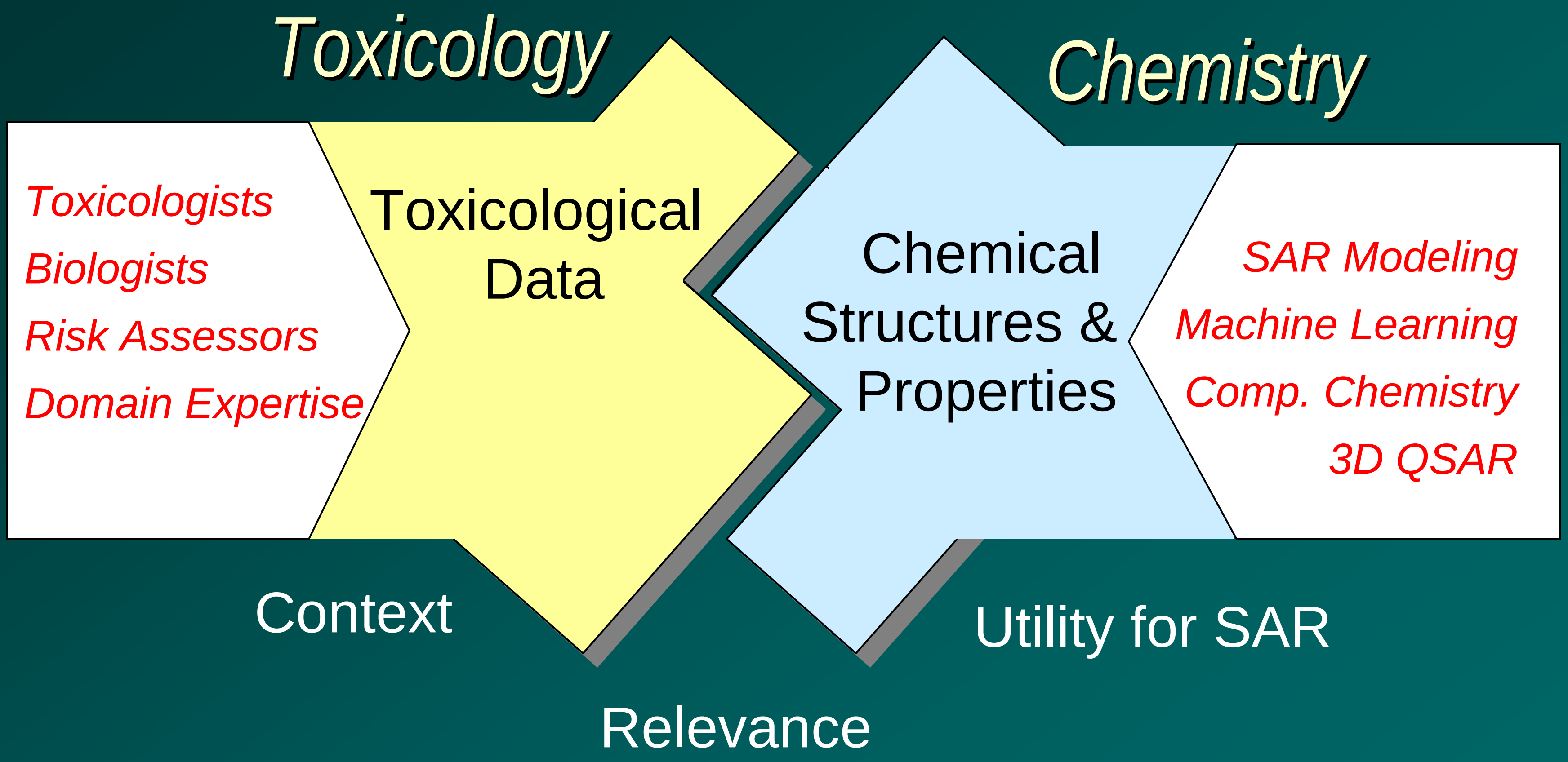
Carcinogenic Potency Database Summary Tables (CPDBAS, CPDBHA, CPDBDG, CPDBPR)

Log File

DSSTox Log File:

Carcinogenic Potency Database Summary Tables (CPDBAS, CPDBHA, CPDBDG, CPDBPR)

DSSTox Database Design:



Toxicology

Toxicologists

Biologists

Risk Assessors

Domain Expertise

Toxicological Data

Context

Chemistry

Chemical Structures & Properties

SAR Modeling

Machine Learning

Comp. Chemistry

3D QSAR

Utility for SAR

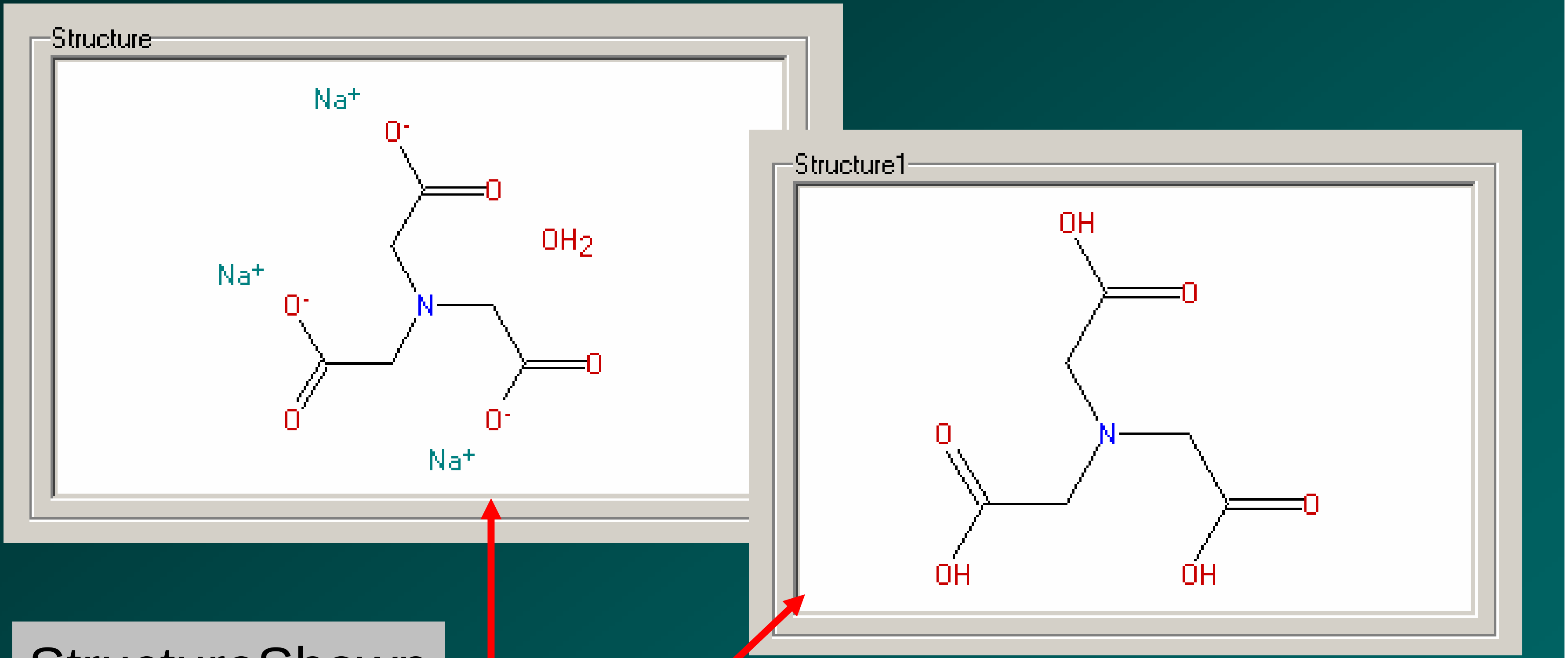
Relevance

DSSTox Toxicity Database Standards:

- Data file format (SDF)
- File naming convention
- Chemical structure information fields
- Documentation requirements
- Publishing requirements

DSSTox Standard Chemical Fields:

- Structure *2D chemical structure*
- StructureShown *Description of displayed 2D structure*
  - ***tested form, simplified to parent, predicted form, active ingredient of formulation, general form***
- Formula *Empirical molecular formula*
- MolWeight *Molecular weight in atomic units*
- CAS *Chem Abstracts Service No. for StructureShown*
- SMILES *Linear text notation for 2D StructureShown*
- DSSTox_ID *Counter allows unique identification of record*
- DSSTox_FileName *Name of file included in each record*
- ChemName *Chemical name from original data base*
- SubstanceType *Broad substance classification*
  - ***defined organic, inorganic, organometallic, polymer, mixture or unknown***
- TestedForm *Tested form of chemical*
  - ***parent, salt, complex, unknown or multiple forms***
- AddToParent *Salt counterions or complexed moieties*
- CAS_TestedForm *CAS No. for tested form of chemical*
- SMILES_TestedForm *SMILES code for the tested form of the chemical*
- ChemNote *Additional qualifier info for chemical fields*
  - ***defined mixture characteristics, uncertainty in structure or CAS, stereochem, replicate, etc.***
- ChemCount *Counter for structure or CAS duplications in db*



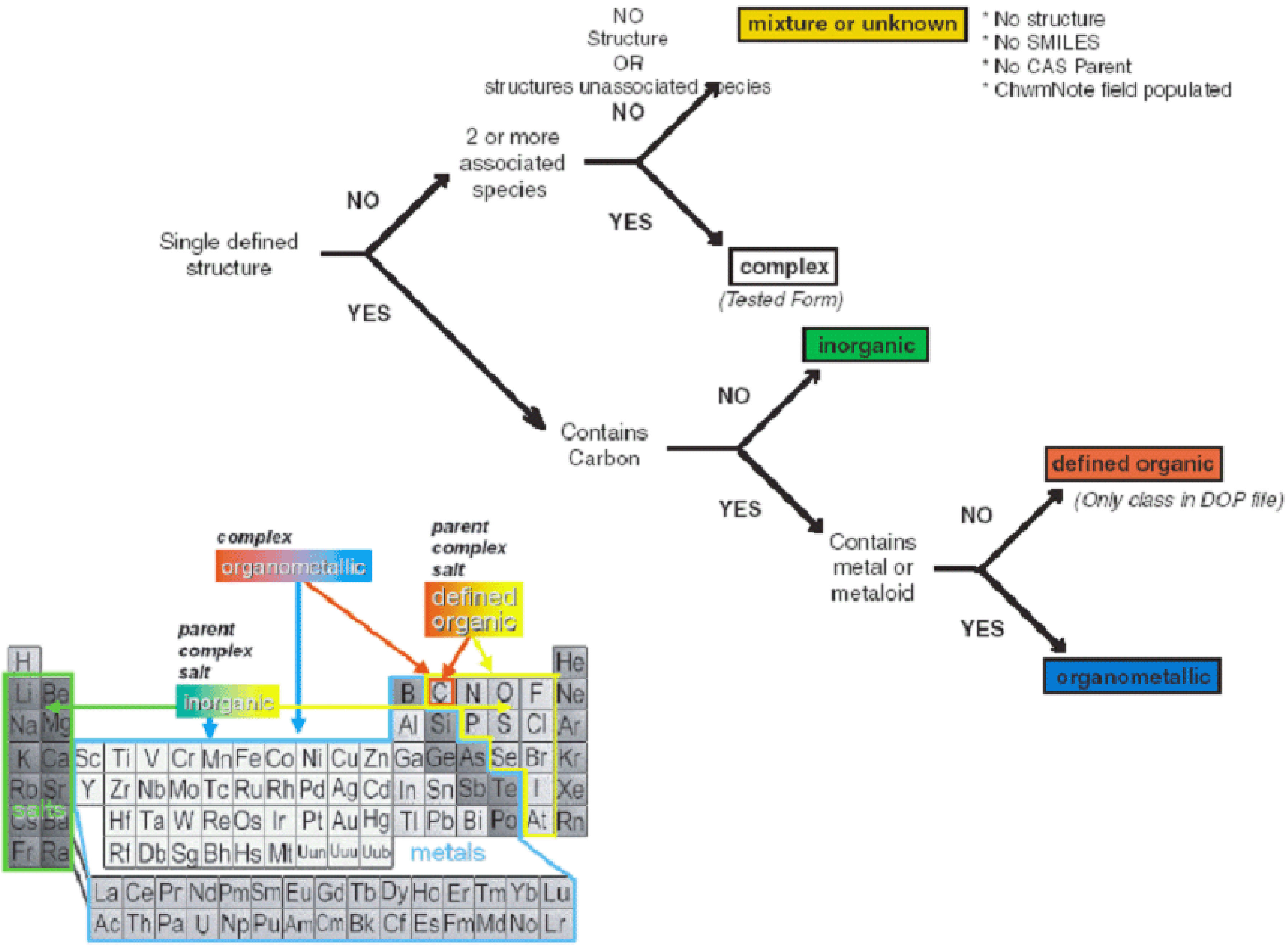
StructureShown

- Tested form
- Simplified to parent
- General form
- Active ingredient of formulation
- Monomer of polymeric form

Linked-content fields

- CAS
- SMILES
- Formula
- MolWt

Substance Type



Single defined structure

NO

2 or more associated species

NO

NO Structure OR structures unassociated species

mixture or unknown

- * No structure
- * No SMILES
- * No CAS Parent
- * ChwmNote field populated

YES

complex

(Tested Form)

YES

Contains Carbon

NO

inorganic

YES

Contains metal or metaloid

NO

defined organic

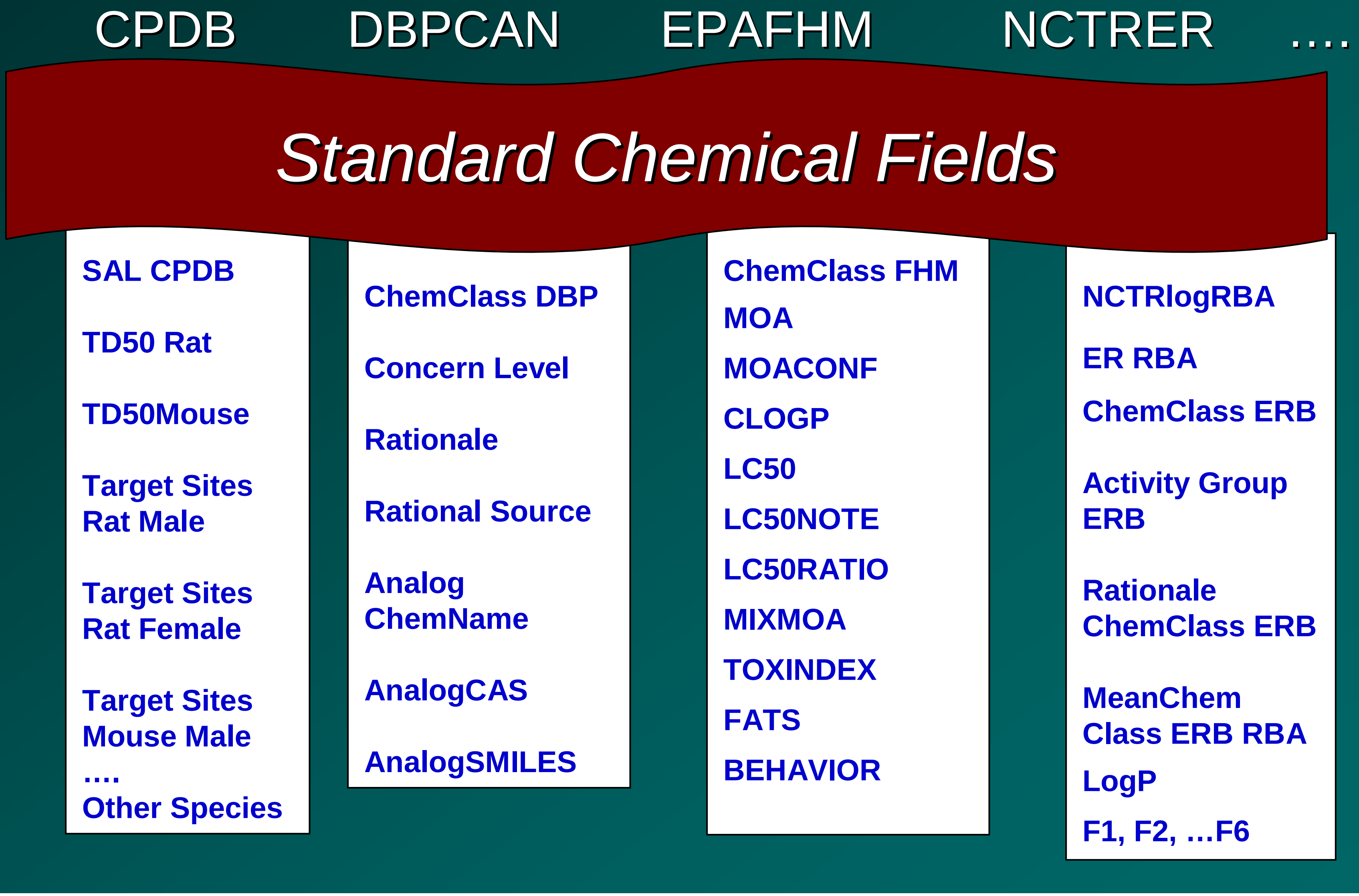
(Only class in DOP file)

YES

organometallic

complex
organometallic
parent complex salt
defined organic
parent complex salt
inorganic
salts
metals
H He
Li Be B C N O F Ne
Na Mg Al Si P S Cl Ar
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
Cs Ba Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
Fr Ra Rf Db Sg Bh Hs Mt Uun Uuu Uub
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu
Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

Integrating Diverse Databases from a Chemical Structure Perspective:



CPDB DBPCAN EPAFHM NCTRER ….

Standard Chemical Fields

CPDB

- SAL CPDB
- TD50 Rat
- TD50Mouse
- Target Sites Rat Male
- Target Sites Rat Female
- Target Sites Mouse Male
- ….
- Other Species

DBPCAN

- ChemClass DBP
- Concern Level
- Rationale
- Rational Source
- Analog ChemName
- AnalogCAS
- AnalogSMILES

EPAFHM

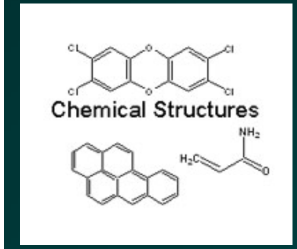
- ChemClass FHM
- MOA
- MOACONF
- CLOGP
- LC50
- LC50NOTE
- LC50RATIO
- MIXMOA
- TOXINDEX
- FATS
- BEHAVIOR

NCTRER

- NCTRlogRBA
- ER RBA
- ChemClass ERB
- Activity Group ERB
- Rationale ChemClass ERB
- MeanChem Class ERB RBA
- LogP
- F1, F2, …F6

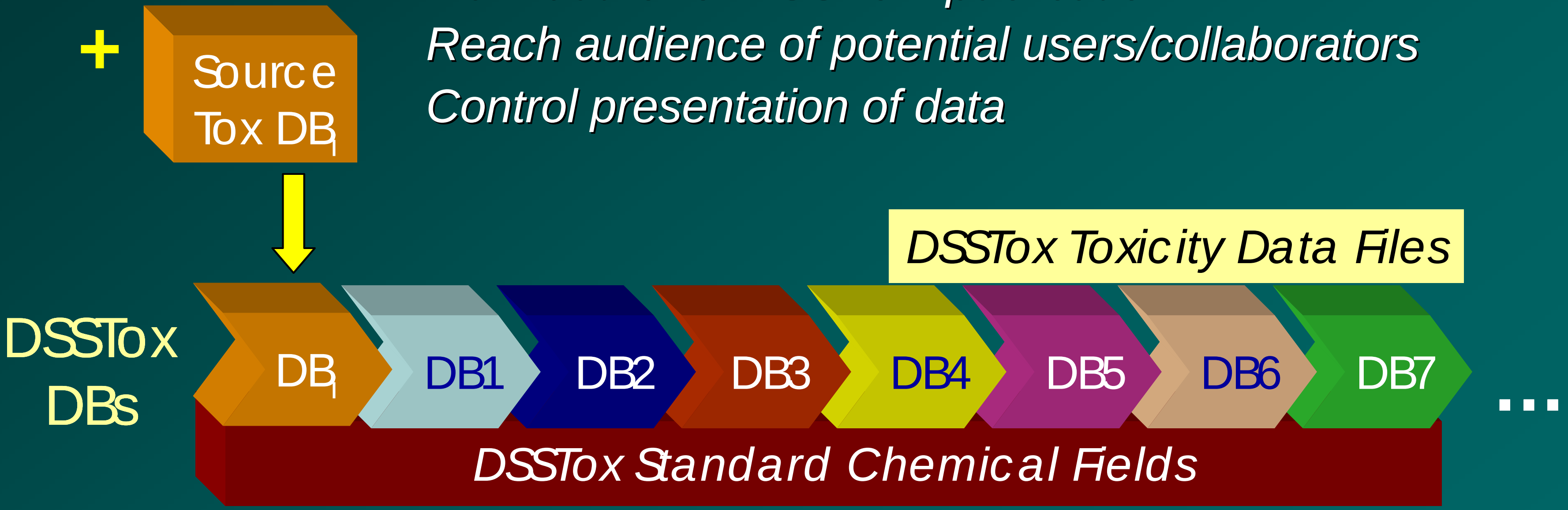
DSSTox Project Feasibility:

Direct Benefits to Data Source Collaborators



Chemical structure annotation
Construct standardized DSSTox data file

Main-author of DSSTox "publication"
Reach audience of potential users/collaborators
Control presentation of data

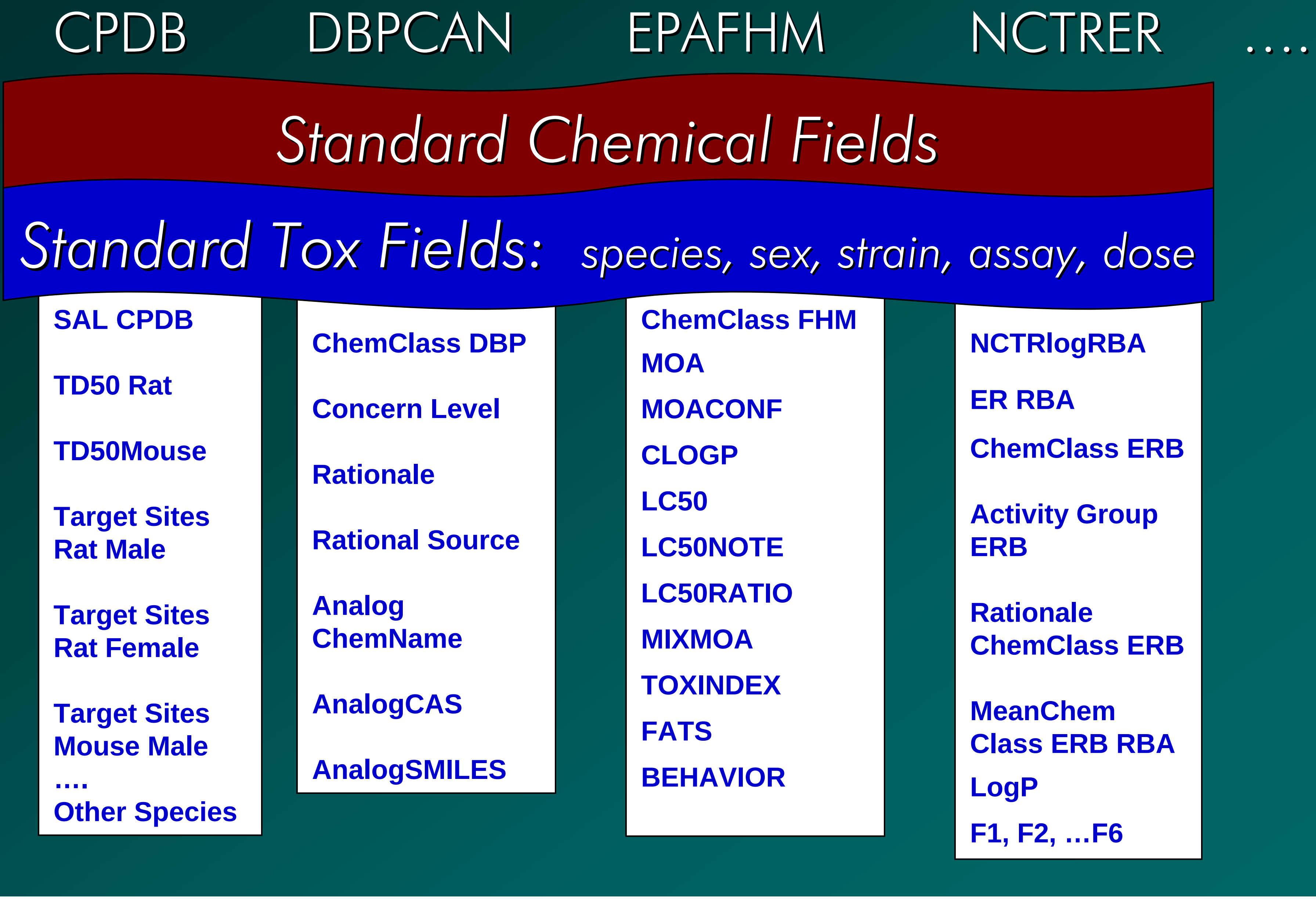


Source DB can now be linked with DSSTox DB library and structure searched.

DSSTox Database Network:

- How can DSSTox files be used?
- What’s next?

Begin to incorporate standard tox fields (ToXML)



CPDB DBPCAN EPAFHM NCTRER ….

Standard Chemical Fields

Standard Tox Fields: species, sex, strain, assay, dose

SAL CPDB

TD50 Rat

TD50Mouse

Target Sites Rat Male

Target Sites Rat Female

Target Sites Mouse Male

….

Other Species

ChemClass DBP

Concern Level

Rationale

Rational Source

Analog ChemName

AnalogCAS

AnalogSMILES

ChemClass FHM

MOA

MOACONF

CLOGP

LC50

LC50NOTE

LC50RATIO

MIXMOA

TOXINDEX

FATS

BEHAVIOR

NCTRlogRBA

ER RBA

ChemClass ERB

Activity Group ERB

Rationale ChemClass ERB

MeanChem Class ERB RBA

LogP

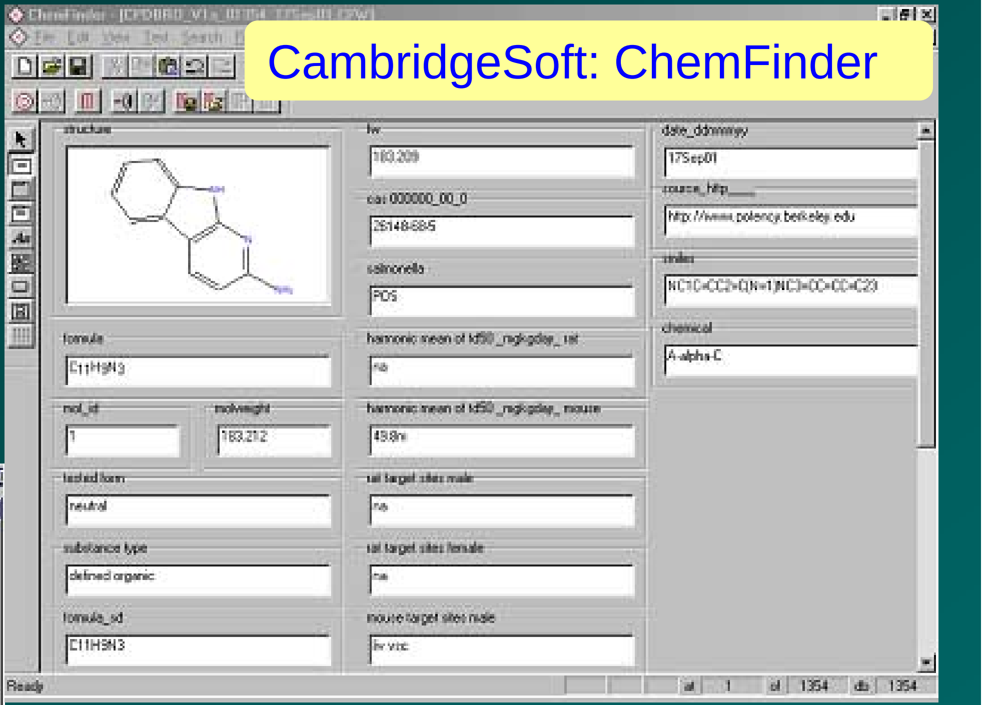
F1, F2, …F6

Migrate More Public Toxicity Data into DSSTox Standard Format: Phase II, III, …

- FDA Max Recommended Therapeutic Dose - Pharmaceuticals
- NCTR Androgen, Thyroid, and Endocrine Disruption Databases
- NTP Rodent carcinogenicity bioassays, subchronic bioassays, developmental, repro, immuno, etc.
- ICVAM databases on LD50, skin sensitization, local lymph node assay, skin corrosivity, endocrine disruption, etc
- EPA pesticide ecotoxicity database
- Developmental toxicity database (literature – FDA,TOPKAT)
- UniLever Skin Sensitization database
- EPA’s High Production Volume (HPV) chemical data
- EPA’s Integrated Risk Information System (IRIS)

Chemical Relational Databases: *Exploration across toxicological domains and structural/biological axes*

Accord
Oracle
ISIS
ChemFolder
ChemFinder
LeadScope
BioRad



CambridgeSoft: ChemFinder

structure

formula: $C_{11}H_9N_3$

mol_id: 1

molweight: 183.212

tested form: neutral

substance type: defined organic

formula_sd: C11H9N3

fw: 183.209

cas 000000_00_0: 26148-68-5

salmonella: POS

harmonic mean of td50_mgkgday_rat: na

harmonic mean of td50_mgkgday_mouse: 49.8m

rat target sites male: na

rat target sites female: na

mouse target sites male: liv vsc

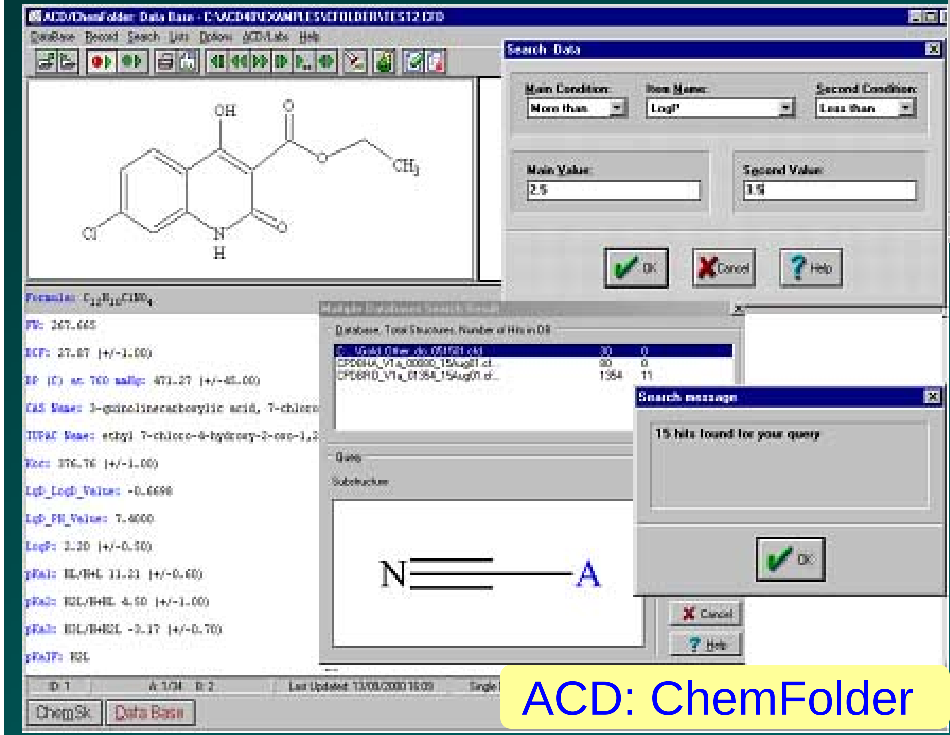
date_ddmmmyy: 17Sep01

source_http: http://www.potency.berkeley.edu

smiles: NC1C=CC2=C(N=1)NC3=CC=CC=C23

chemical: A-alpha-C

Ready



Formula: $C_{12}H_{10}ClNO_4$

FW: 267.665

BCF: 27.87 (+/-1.00)

BP (C) at 760 mmHg: 471.27 (+/-45.00)

CAS Name: 3-quinolinecarboxylic acid, 7-chloro

IUPAC Name: ethyl 7-chloro-4-hydroxy-2-oxo-1,2

Koc: 376.76 (+/-1.00)

Lgb_LogD_Value: -0.6698

Lgb_PH_Value: 7.4000

LogP: 2.20 (+/-0.50)

pKa1: HL/H+L 11.21 (+/-0.60)

pKa2: H2L/H+HL 4.50 (+/-1.00)

pKa3: H3L/H+H2L -3.17 (+/-0.70)

pKaTP: H2L

Search Data

Main Condition: More than
Item Name: LogP
Second Condition: Less than
Main Value: 2.5
Second Value: 1.5

Database, Total Structures, Number of Hits in DB

C:...\Gold Other_db_051501.cfd	30	0
CPDBHA_V1a_00000_15Aug01.cf...	80	0
CPDB810_V1a_01384_15Aug01.cf...	1384	11

Query
Substructure

Search message

15 hits found for your query

ACD: ChemFolder

Freeware SDF Viewer Application

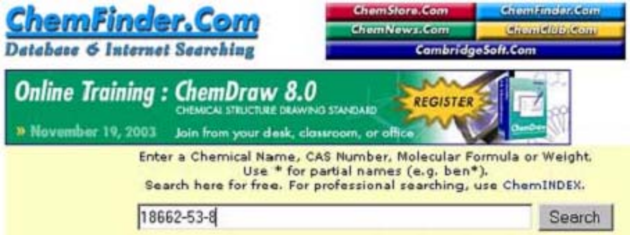
Non-EPA on-line structure searching

EPA on-line structure searching

Coordinating Public Efforts:

DSSTox COMMUNITY

- ACD/Labs (Advanced Chemistry Development) ChemFolder Public Databases
- Cambridge-Soft's ChemFinder.Com Chemical Search Website
- FDA (Food & Drug Administration) Center for Drug Evaluation & Research
- ILSI (International Life Sciences Institute) SAR Toxicity Database Project, in collaboration with LHASA, Lmt.LIST (LeadScope In Silico Tox) Focus Group
- LIST (LeadScope In Silico Tox) Focus Group
- MGED: MIAMI-Tox
- NCI (National Cancer Institute) Public Data Outreach – Structure Web Browser
- NIEHS's National Center for Toxicogenomics
- NLM (National Library of Medicine) TOXNET
- NTP (National Toxicology Program) On-line Public Databases
- SRC (Syracuse Research Corporation) PBT-Profiler and Analog Search Tools


ChemFinder.Com
Database & Internet Searching
ChemStore.Com
ChemFinder.Com
ChemNews.Com
ChemClub.Com
CambridgeSoft.Com
Online Training : ChemDraw 8.0
CHEMICAL STRUCTURE DRAWING STANDARD
» November 19, 2003
Join from your desk, classroom, or office
REGISTER
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Enter a Chemical Name, CAS Number, Molecular Formula or Weight.
Use * for partial names (e.g. ben*).
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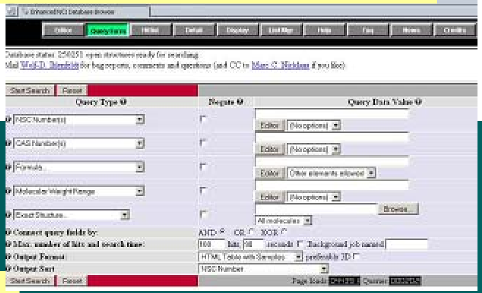
18662-53-8

NCI Structure-Browser



Database status: 250251 open structures ready for searching
Mail Wolf-D. Ihlenfeldt for bug reports, comments and questions (and CC to Marc C. Nicklaus if you like)

Query Type	Negate	Query Data Value
NSC Number(s)	☐	(No options)
CAS Number(s)	☐	(No options)
Formula	☐	Other elements allowed
Molecular Weight Range	☐	(No options)
Exact Structure...	☐	All molecules

Connect query fields by: AND ● OR ○ XOR ○
Max. number of hits and search time: 100 hits 50 seconds ☐ Background job named
Output Format: HTML Table with Samples ☐ preferably 3D
Output Sort: NSC Number

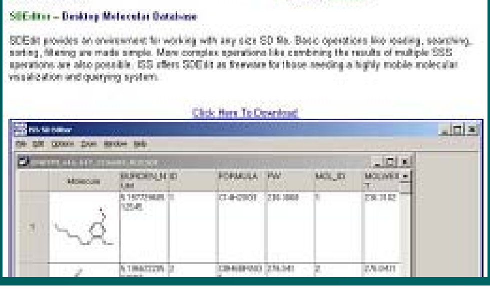
Advanced Chemistry Development

Web Librarian DBs

We have made the numerous DSSTox databases available in a number of flexible formats. Below are listed four links for each database.

- The **DSSTox description link** will take you directly to the DSSTox webpage from which the source files are obtained and where any modifications to the databases will be made available.
- The **SDF file link** will enable you to download these files directly from the DSSTox website.
- The **CFD file** includes the source files in ChemFolder format and a ChemFolder form to use with the database for more visual appeal.
- The **online database links** provide direct online access to the databases via our ACD/Web Librarian interface. This interface allows structure, substructure and alphanumeric text based searching of the databases. For details of how to use the system please review the online help file indicated by the at the top right hand side of the page.

ISSCentral – Freeware CRD



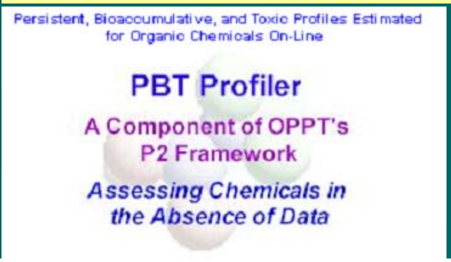
SDEditor – Desktop Molecular Database

SDEdit provides an environment for working with any size SD file. Basic operations like loading, searching, sorting, filtering are made simple. More complex operations like combining the results of multiple SSS operations are also possible. ISS offers SDEdit as freeware for those needing a highly mobile molecular visualization and querying system.

Click Here To Download

	Molecule	BURDEN_N ID LIM		FORMULA	FW	MOL_ID	MOLWEIGHT
1		[illegible]	1	[illegible]	[illegible]	1	[illegible]
		[illegible]	2	[illegible]	[illegible]	2	[illegible]

EPA/Syracuse Res Corp



Persistent, Bioaccumulative, and Toxic Profiles Estimated for Organic Chemicals On-Line

PBT Profiler

A Component of OPPT's P2 Framework

Assessing Chemicals in the Absence of Data

Collaboration with NIEHS/National Center for Toxicogenomics: *Chemical Effects in Biological System Knowledge-Base (CEBS)*

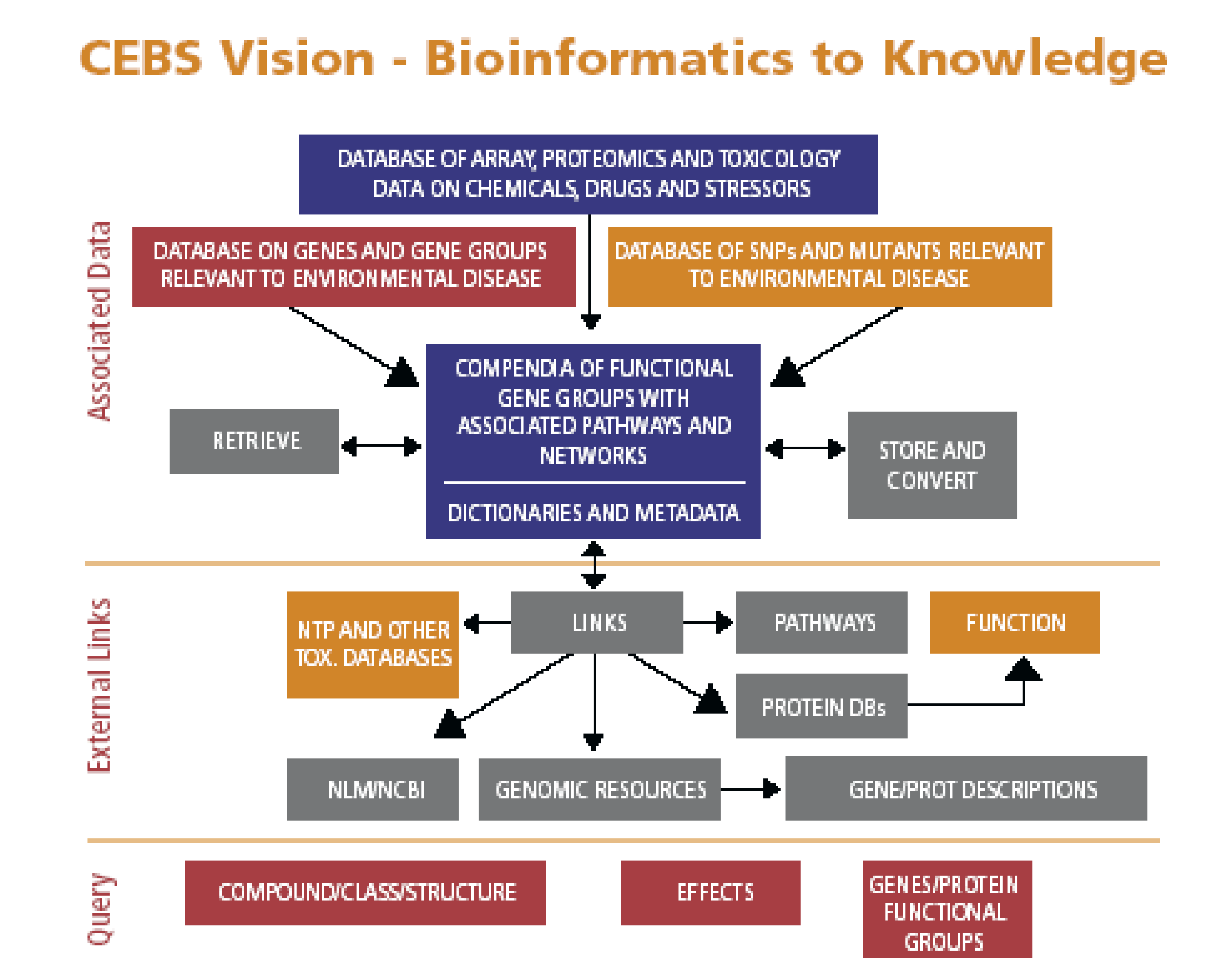
Gene expression

Gene Pathways

Gene Function

Proteomics

Historical Toxicity data



CEBS Vision - Bioinformatics to Knowledge

Associated Data

DATABASE OF ARRAY, PROTEOMICS AND TOXICOLOGY DATA ON CHEMICALS, DRUGS AND STRESSORS

DATABASE ON GENES AND GENE GROUPS RELEVANT TO ENVIRONMENTAL DISEASE

DATABASE OF SNPs AND MUTANTS RELEVANT TO ENVIRONMENTAL DISEASE

RETRIEVE

COMPENDIA OF FUNCTIONAL GENE GROUPS WITH ASSOCIATED PATHWAYS AND NETWORKS

DICTIONARIES AND METADATA

STORE AND CONVERT

External Links

NTP AND OTHER TOX. DATABASES

LINKS

PATHWAYS

FUNCTION

PROTEIN DBs

NLM/NCBI

GENOMIC RESOURCES

GENE/PROT DESCRIPTIONS

Query

COMPOUND/CLASS/STRUCTURE

EFFECTS

GENES/PROTEIN FUNCTIONAL GROUPS

Collaboration with NIEHS/National Center for Toxicogenomics: *Chemical Effects in Biological System Knowledge-Base (CEBS)*

DSSTox +

Gene expression

Gene Pathways

Gene Function

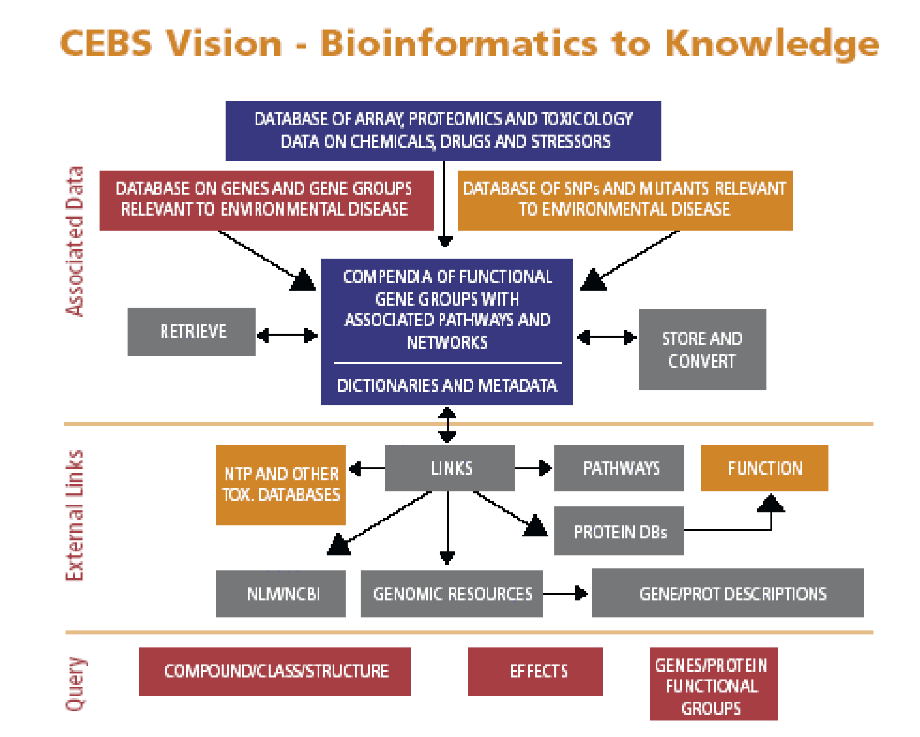
Proteomics

Historical Toxicity data

DSSTox Toxicity Data Files

DB1 DB2 DB3 DB4 DB5 DB6 DB7

DSSTox Standard Chemical Fields

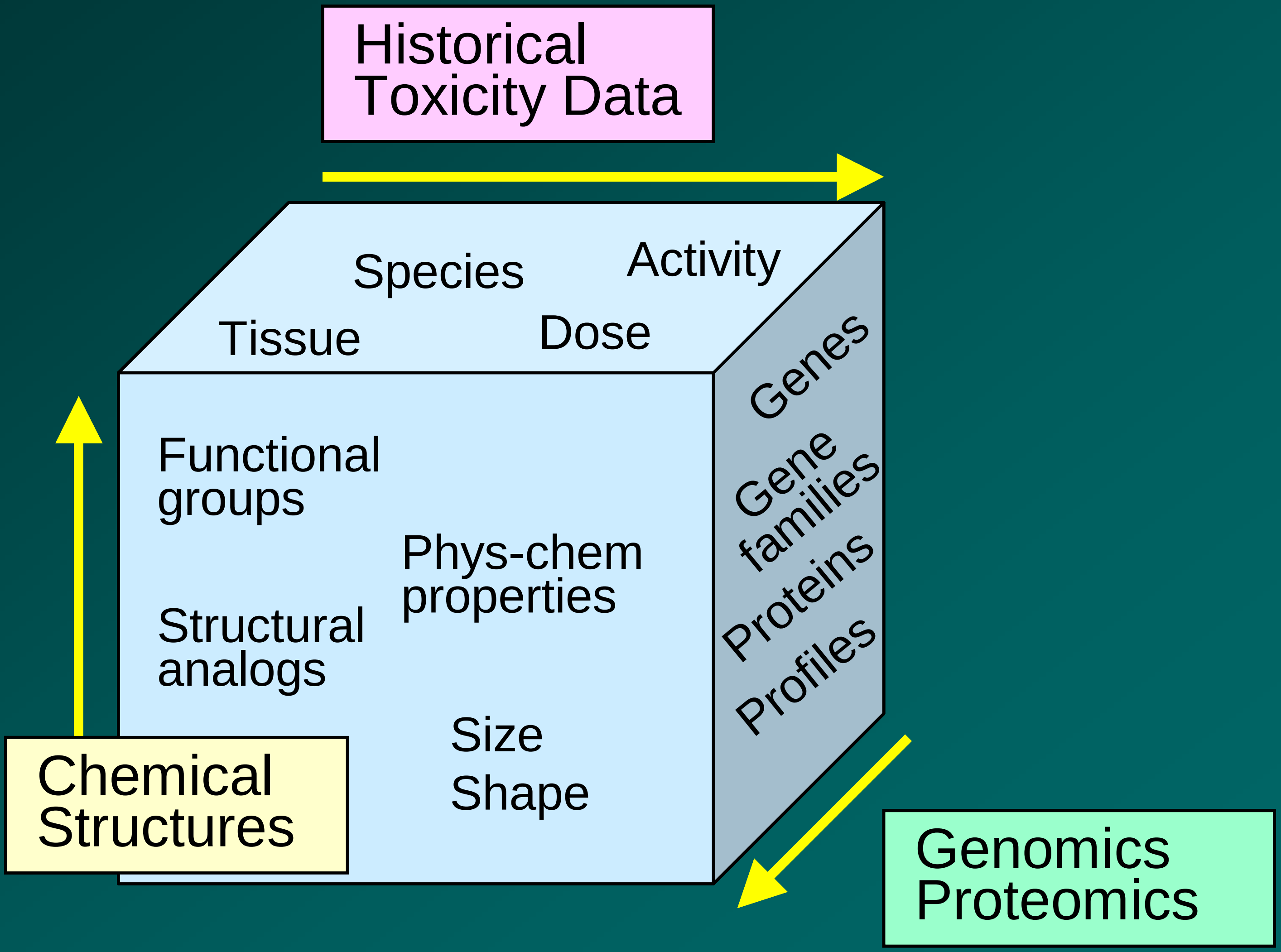


CEBS Vision - Bioinformatics to Knowledge

Associated Data
DATABASE OF ARRAY, PROTEOMICS AND TOXICOLOGY DATA ON CHEMICALS, DRUGS AND STRESSORS
DATABASE ON GENES AND GENE GROUPS RELEVANT TO ENVIRONMENTAL DISEASE
DATABASE OF SNPs AND MUTANTS RELEVANT TO ENVIRONMENTAL DISEASE
RETRIEVE
COMPENDIA OF FUNCTIONAL GENE GROUPS WITH ASSOCIATED PATHWAYS AND NETWORKS
DICTIONARIES AND METADATA
STORE AND CONVERT
External Links
NTP AND OTHER TOX. DATABASES
LINKS
PATHWAYS
FUNCTION
PROTEIN DBs
NLM/NCBI
GENOMIC RESOURCES
GENE/PROT DESCRIPTIONS
Query
COMPOUND/CLASS/STRUCTURE
EFFECTS
GENES/PROTEIN FUNCTIONAL GROUPS

Chemo-bioinformatics:

Expanded Relational Search Domains



DSSTox Public Toxicity Data Network

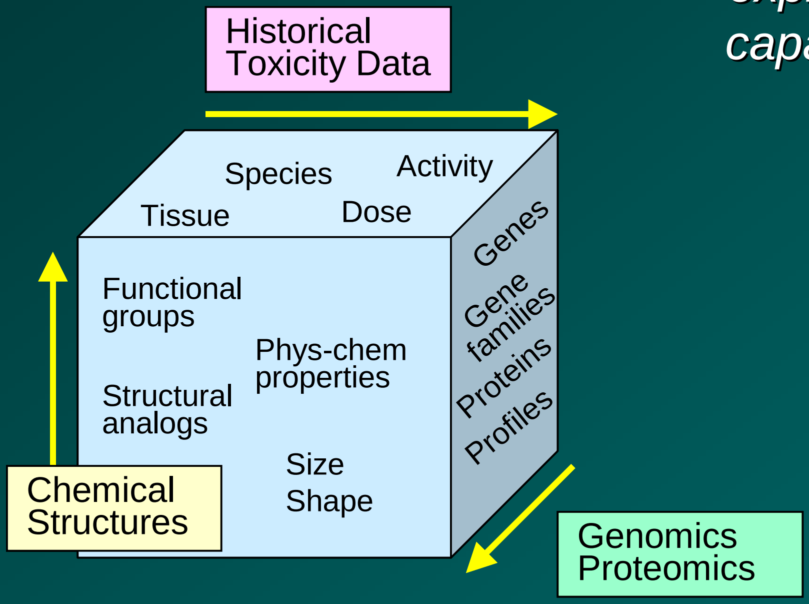
- Structural Annotation
- File standardization
- Standardized fields
- Documentation
- Quality review

Improved data exploration capabilities

Relational searching capability across information domains

Improved biofunctional classifications

Improved SAR models



Adoption of DSSTox data/file standards

Improved public access to toxicity data

DSSTox

Increased use of chemical structure searching

Improved toxicity predictions

DSSTox Collaborators/Advisors/Acknowledgements:

Cancer Potency Data Base - rodent carcinogenicity	Lois Swirsky Gold, Thomas Slone
EPA - Ecotoxicity (fathead minnow, Teratox)	Chris Russom
EPA/OPPT,OW – DBP cancer assessment	Yin-tak Woo, Mary Manibusan
FDA/NCTR - Estrogen receptor binding data base	Weida Tong, Hong Fang
FDA/CDER – Maximum recommended dose drugs	Dan Benz, Ed Matthews, Joe Contrera
EPA/OPP, Ecotox – pesticides	Brian Montague, Pauline Wagner
NTP Gene-tox data; IRIS	Errol Zeiger, Zeiger Consulting
Nat Ctr Toxicogenomics: CEBS	Mike Waters, Ray Tennant
GlaxoSK - GeneTox/NTP Salmonella database	Neal Cariello, Vijay Gombar
NIEHS/NTP Rodent carcinogenicity, etc	Skip Eastin, Doug Bristol
Developmental toxicity	Vijay Gombar (GlaxoSK), Orest Macina
ICVAM Toxicity databases	Ray Tice, Marc Jackson, ILS
Unilever Skin Sensitization Database	Martin Barrett, Marlin Consulting
ZEBET Acute Toxicity Database	Julie Penzotti, Rational Discovery
Tulane/Xavier Univ – Endocrine Disruption	Tom Wiese
NCI – SDF tools, CACTVS structure browser	Marc Nicklaus
LeadScope – SDF/XML converter, FDA carcinogens	Chihae Yang
SDF Viewer application	Thomas Harrocks, Intuitive Software Solutions
ACD – ChemFolder, WebBase	Antony Williams, M Hachey, G Shear
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